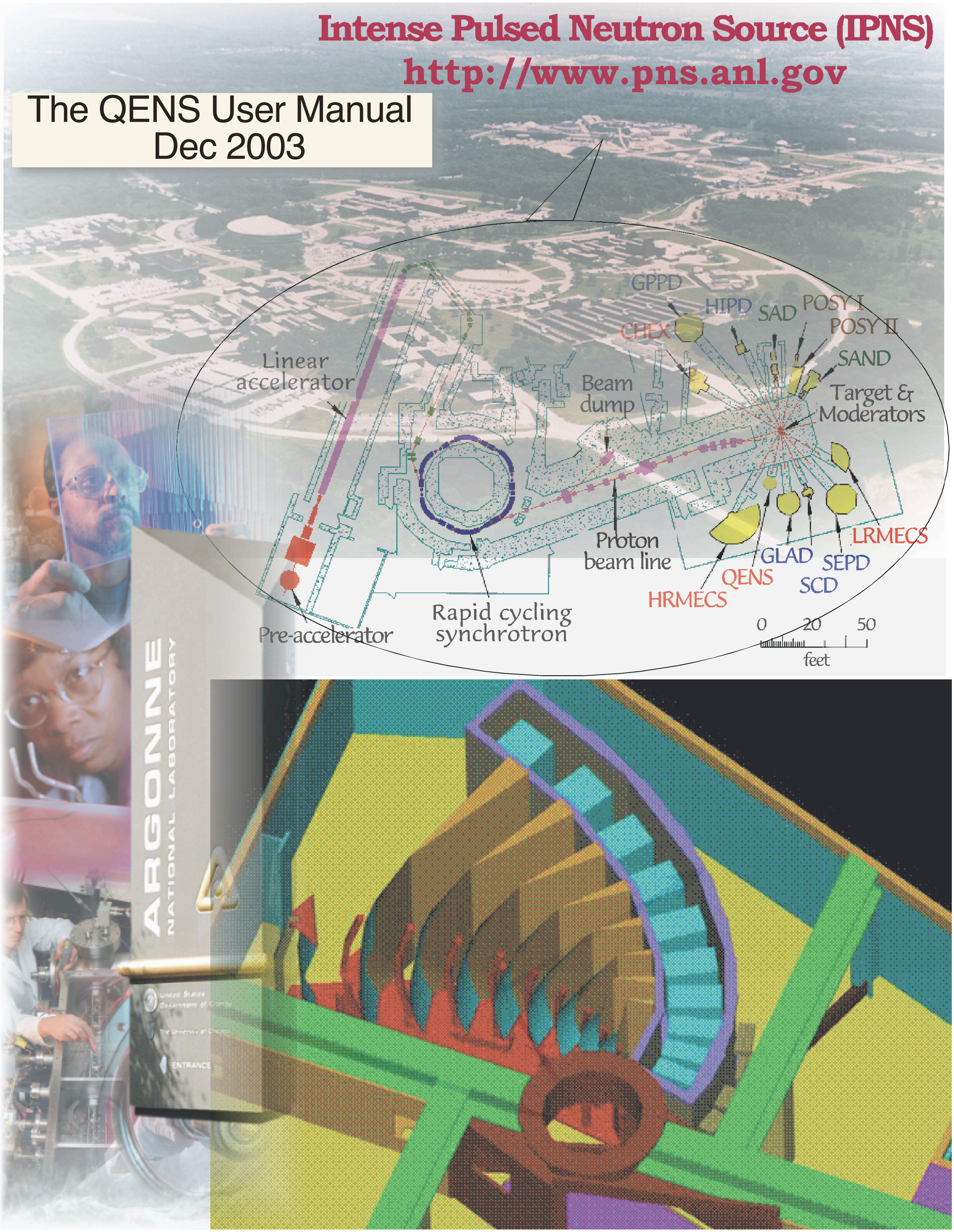
Intense Pulsed Neutron Source (IPNS)

http://www.pns.anl.gov

The QENS User Manual
Dec 2003



Content

QENS Contacts 3

A Brief History 4

Instrument

Layout 5

Analyzer-Detector Configuration 6

(Q,E)-Coverage & Energy Resolution 7

Sample Environment 8

Data Acquisition System 10

Data Reduction & Analysis

QENS Data Reduction & Analysis 11

Check Inelastic Data 12

Calibration and Normalization of Inelastic Data 13

Convert, Integrate, and Overplot Inelastic Datasets 14

Check Diffraction Data 15

View & Overplot Diffraction Data 16

ASCII Files of Diffraction & Inelastic Data 17

Welcome to the QuasiElastic Neutron Spectrometer (QENS)

This user manual is meant to assist you - the QENS valued customers - to conduct experiments on QENS. We hope to provide the accurate and current information. You are the best person to decide if the manual is useful or needs improvements. Please contact us.

QENS Contacts

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QENS Passwords

Please ask us

A Brief History of QENS

QENS is the result of a combined effort of many contributors. At the outset it has been a user instrument. The experience of interacting with numerous users for almost two decades has provided valuable guidance for the in-house staff to enhance QENS scientific capabilities. Some key milestones of improvement are:

1986 QENS was commissioned following the retirement of an earlier Crystal Analyzer Spectrometer (CAS). It featured three detector arms, housing a total of 35 ^{3}He detectors. Only a small portion of the scattering angles was covered at each setting. Collection of data over the full Q-range required several measurements each conducted at a different scattering angle setting by rotating the entire detector-arm unit.

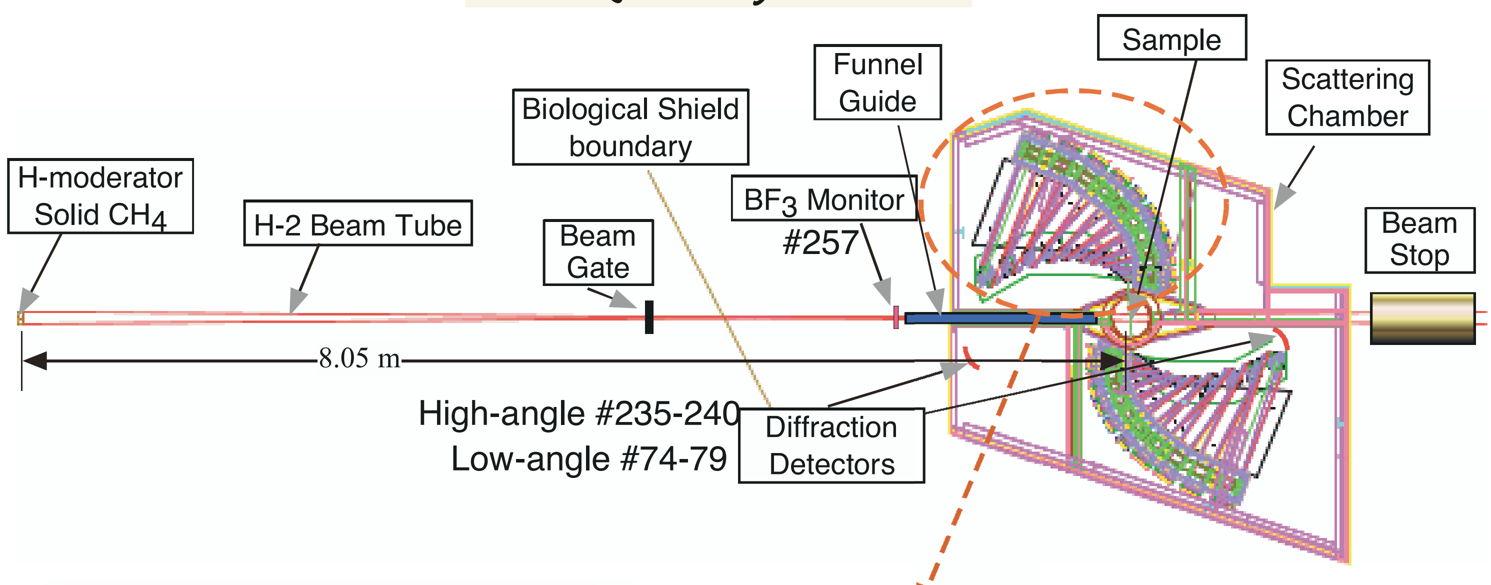
2001 QENS was completely rebuilt and commenced user operation. It includes 22 crystal-analyzer-detector arms outfitted with cooled beryllium-filters in a new scattering chamber. An average energy resolution (FWHM) varying from 80 meV (elastic) to 4-5% of the energy transfer (inelastic, up to ~200 meV neutron energy loss) was realized over a wide range of wavevectors from 0.3 to 2.5 $Å^{-1}$. Two additional detector clusters enabled concurrent measurements of diffraction patterns from 0.1 to 30 $Å^{-1}$. Because of the substantial reconstruction resulting in significant enhancement, we often refer the present instrument as the "New QENS".

2003 A supermirror, funnel guide was installed in the incident flight path upstream of the sample, resulted in a neutron-flux gain factor of 2.5 (for 5Å-neutrons at sample position).

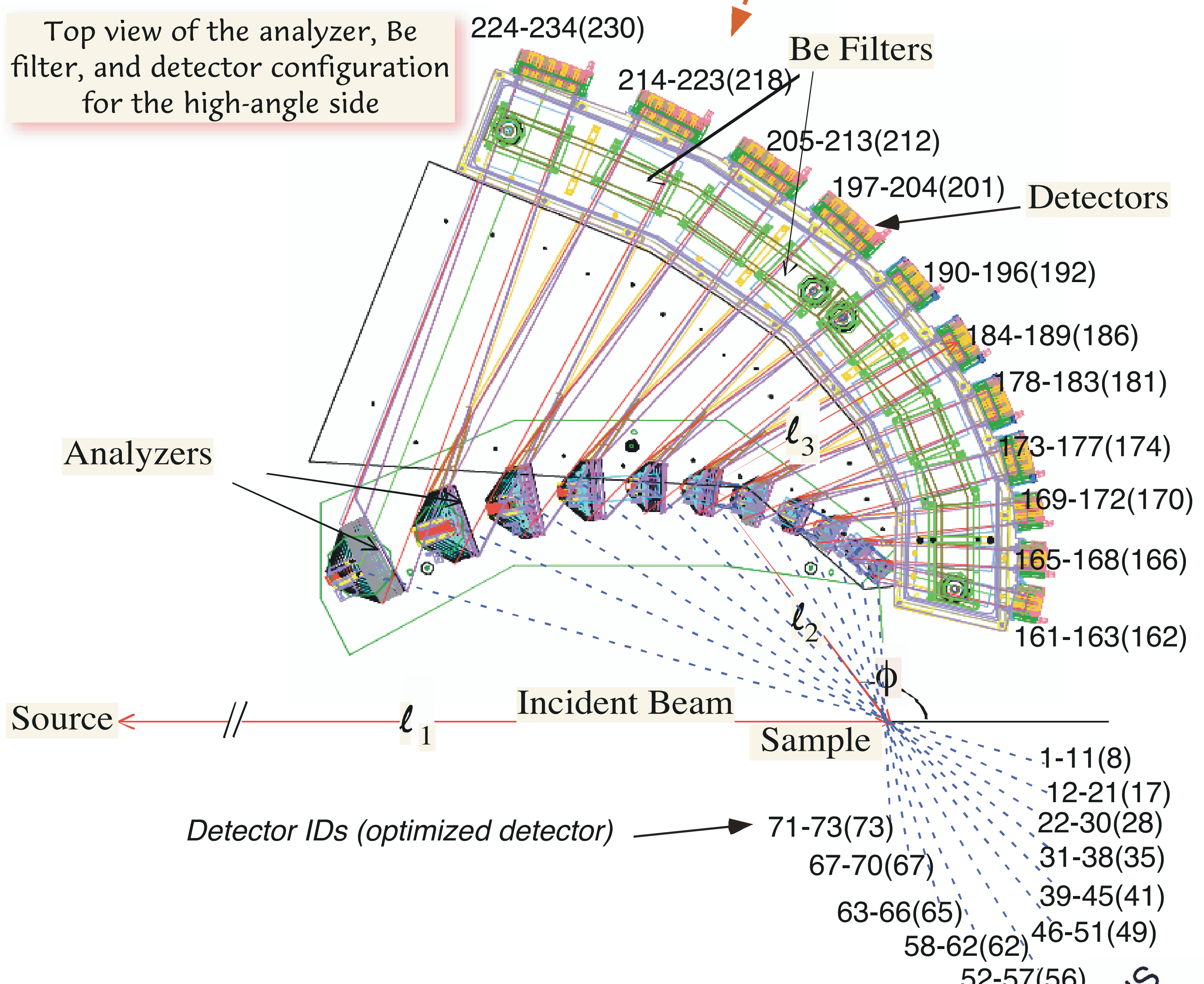
References:

1. K. F. Bradley, S.-H. Chen, T. O. Brun, R. Kleb, W. A. Loomis, and J. M. Newsam, *Nucl. Instr. Methods*, **A270**, 78 (1988).
2. R. K. Crawford, F. Trouw, and H. A. Belch, IPNS Notes No. 79 (1997), unpublished.
3. R. W. Connatser, Jr., H. Belch, L. Jirik, D. J. Leach, F. R. Trouw, J.-M. Zanotti, Y. Ren, R. K. Crawford, J. M. Carpenter, D. L. Price, C.-K. Loong, J. P. Hodges, and K. W. Herwig, in *16th Meeting of the International Collaboration on Advanced Neutron Sources*, edited by G. Mank and H. Conrad (Forschungszentrum Jülich GmbH, Jülich, Germay, Düsseldorf-Neuss, Germany, 2003), Vol. I, p. 279.
4. QENS web page http://www.pns.anl.gov/instruments/qens/

QENS Layout



Sample
Scattering Chamber
Funnel Guide
Biological Shield boundary
BF3 Monitor #257
H-moderator Solid CH4
H-2 Beam Tube
Beam Gate
Beam Stop
8.05 m
High-angle #235-240
Low-angle #74-79
Diffraction Detectors



Top view of the analyzer, Be filter, and detector configuration for the high-angle side
224-234(230)
214-223(218)
Be Filters
205-213(212)
197-204(201)
Detectors
190-196(192)
184-189(186)
178-183(181)
173-177(174)
169-172(170)
165-168(166)
161-163(162)
Analyzers
ℓ_3
ℓ_2
ϕ
Source
ℓ_1
Incident Beam
Sample
Detector IDs (optimized detector)
1-11(8)
12-21(17)
22-30(28)
31-38(35)
39-45(41)
46-51(49)
52-57(56)
58-62(62)
63-66(65)
67-70(67)
71-73(73)

QENS Analyzer-Detector Configuration

Table 1: Parameters for the analyzer-detector arms of QENS

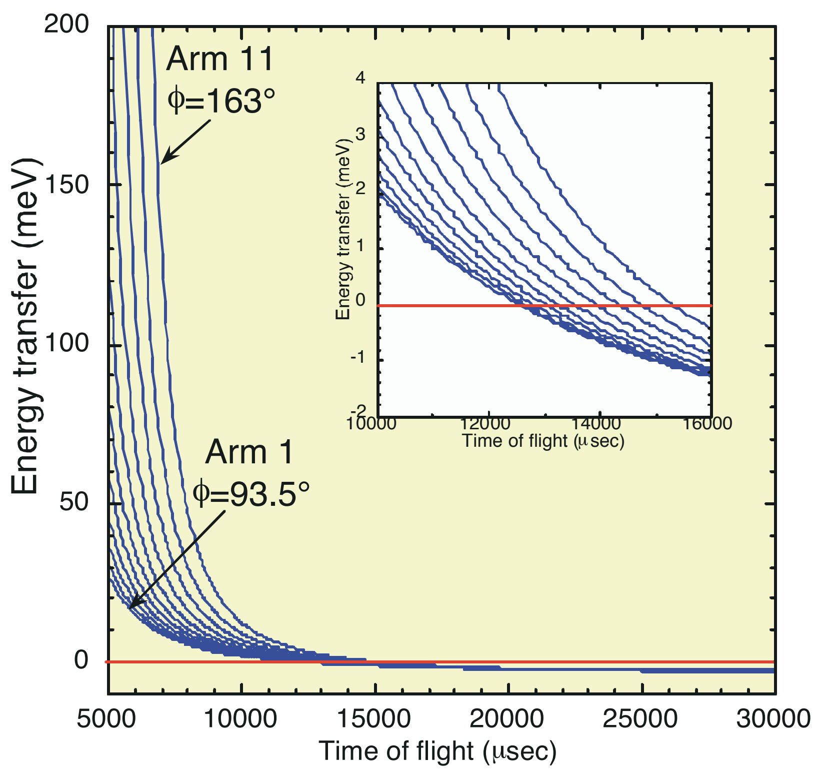
Arm[$]	φ(°)	$\ell_2 = \ell_3$ (m)	θ_B (°)	E_f (meV)	Analyzer area (cm^2)	No. ^3He counters*
1	93.5	0.61	53.7	2.83	74	3
2	100.5	0.70	52.1	2.95	99	4
3	107.5	0.81	51.0	3.04	167	4
4	114.5	0.92	50.2	3.11	185	5
5	121.5	1.05	49.6	3.17	271	6
6	128.5	1.19	49.0	3.23	296	6
7	135.5	1.35	48.5	3.28	345	7
8	142.5	1.53	48.1	3.32	469	8
9	149.5	1.73	47.7	3.37	629	9
10	156.5	1.94	47.3	3.41	740	10
11	163.5	2.19	47.0	3.44	907	11

*Cylindrical tube: ID = 6.4mm, height = 12.7cm, He pressure = 10 atm.

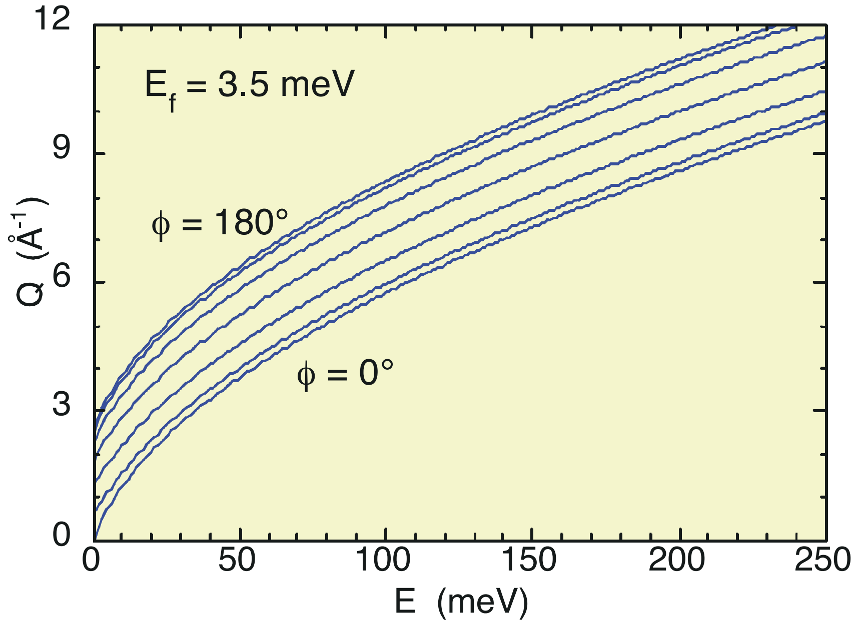
[$]Same parameters for corresponding arms at scattering angles 180°-φ.

Energy transfer E as a function of flight time at detector t: $$E = E_i - E_f = E_f\left(\frac{l_1}{l_2 + l_3}\right)^2\left(\frac{t}{l_2 + l_3}\sqrt{\frac{2E_f}{m_n}} - 1\right)^{-2} - E_f$$

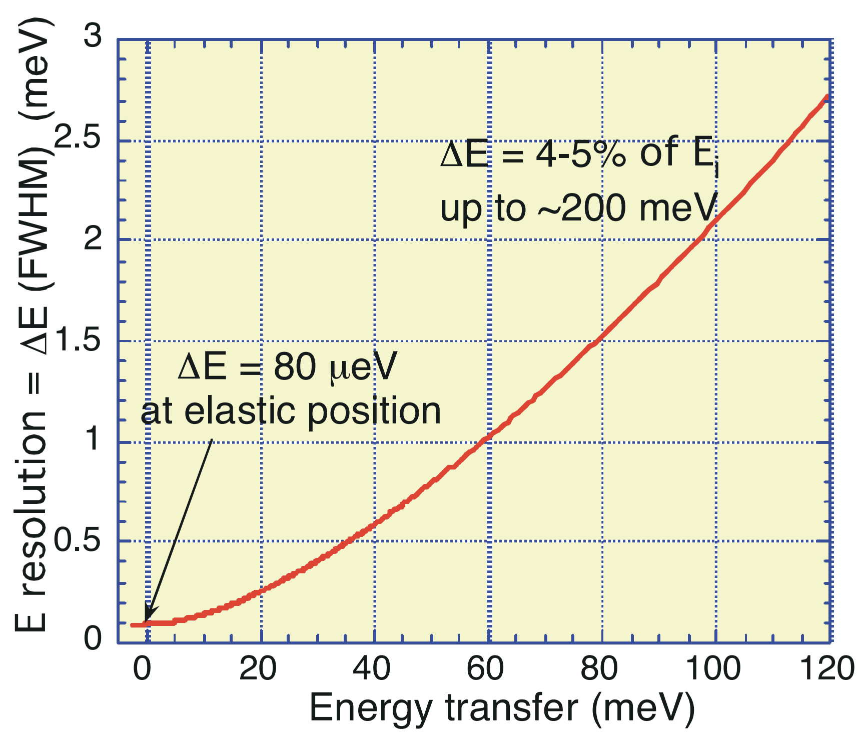
Note that the TOF at a fixed energy, say the elastic channel, differ for different detector arms. Therefore, it is imperative to measure a vanadium standard for each experiment. The vanadium data will be used to calibrate the energy scale for all the detectors and to normalize the spectra against the incident flux distribution. Do make sure the diffraction detectors are working properly.



(Q,E)-Coverage



Energy Resolution



Sample environment

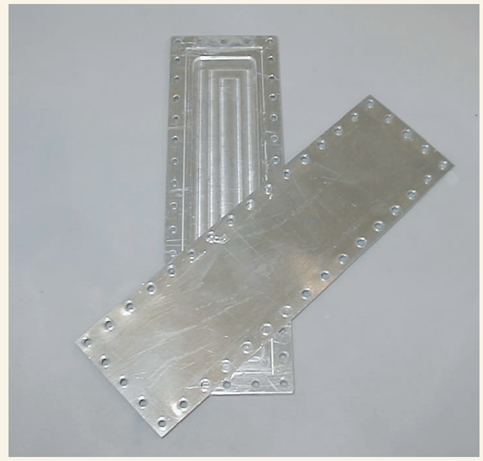
The beam size defined by the funnel guide at the sample position is 3 inches tall by 0.5 inches wide (76mm x 12.5mm). The beam center is 12 inches below the vacuum seal O-ring surface of the sample well. Currently, we are using the sample cans made for the prior beam height of 4 inches.

Ancillary equipments for computer-controlled sample environments:

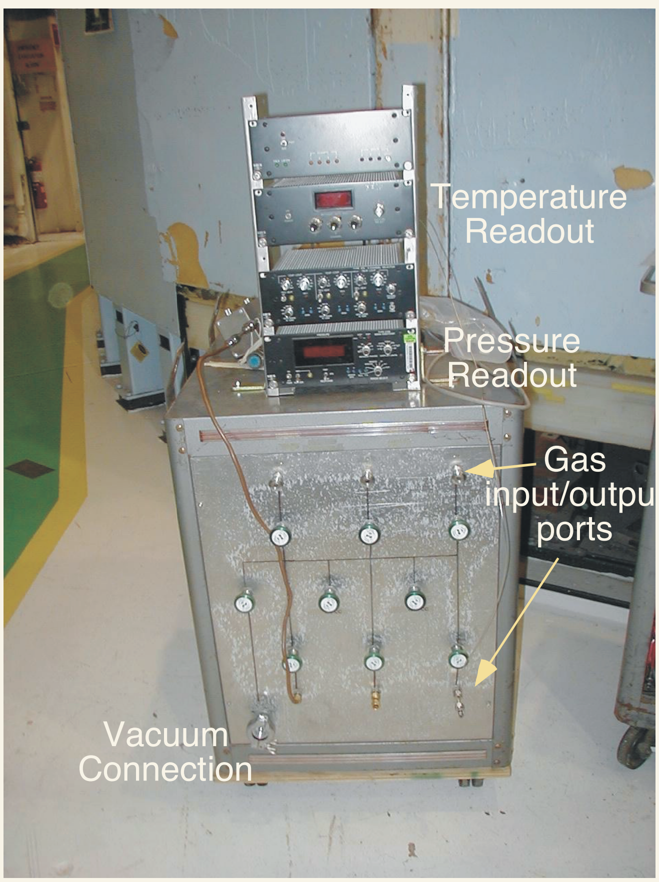
- Room Temperature Mount
- Instrument Displex: 10-300K
- Hot Stage Displex II: 20K-800K
- Orange Cryostat (50mm diameter bore): 1.5K - 300K
- Orange Cryostat (100mm diameter bore): 1.5K - 300K
- Howe Furnace: RT- 1100ºC in vacuum
- Gas handling system for condensing gas molecules in samples

Sample geometry: cylindrical, annular, or flat-plate type. Sample cells are usually made of aluminum alloy and sealed at one end with an indium ring.

Cylindrical cells of id's of 0.125, 0.25 and 0.6 inches are available. Shown here are some of the cylindrical cells for the Displexes and cryostats. *In-situ* gas loading is possible for cylindrical cells.



The annular cell is formed by fitting an inner cylinder into a larger one. Cells of total thickness in the beam of 0.1, 1.0, 1.5 and 2.0 mm are available for use of a Displex. Flat-plate cells of thickness of 0.2, 1.0 and 2.0 mm are available for the Displexes and cryostats.



Typically, gas is delivered via a capillary line from the gas handling system through the Displex mounting plate to the sample cell. Prior to gas loading the system is to be leak checked and pumped out thoroughly. The gas from a known volume at a specific pressure and temperature is expanded into the delivery system and absorbed into the sample while cooling.

Data Acquisition System

At present QENS is operated using a VAX station as the front-end computer under the IPNS first-generation data acquisition system (DAS). Communication with the VAX is usually conducted via a terminal-emulation software (e.g, VersaTerm or Exceed) or by Telnet through the local network. Run setup and sample environment control, etc. are entered by line commands. Live run and data archive are viewed in a graphic window one detector at a time. For example, `dis` displays the spectrum of a detector and `cvs` clears the display. Do not leave the displays on unattended because over a long period of time it may tie up the computer system and disable all communications. Always clear the video screen display by entering `cvs` before leaving the terminal.

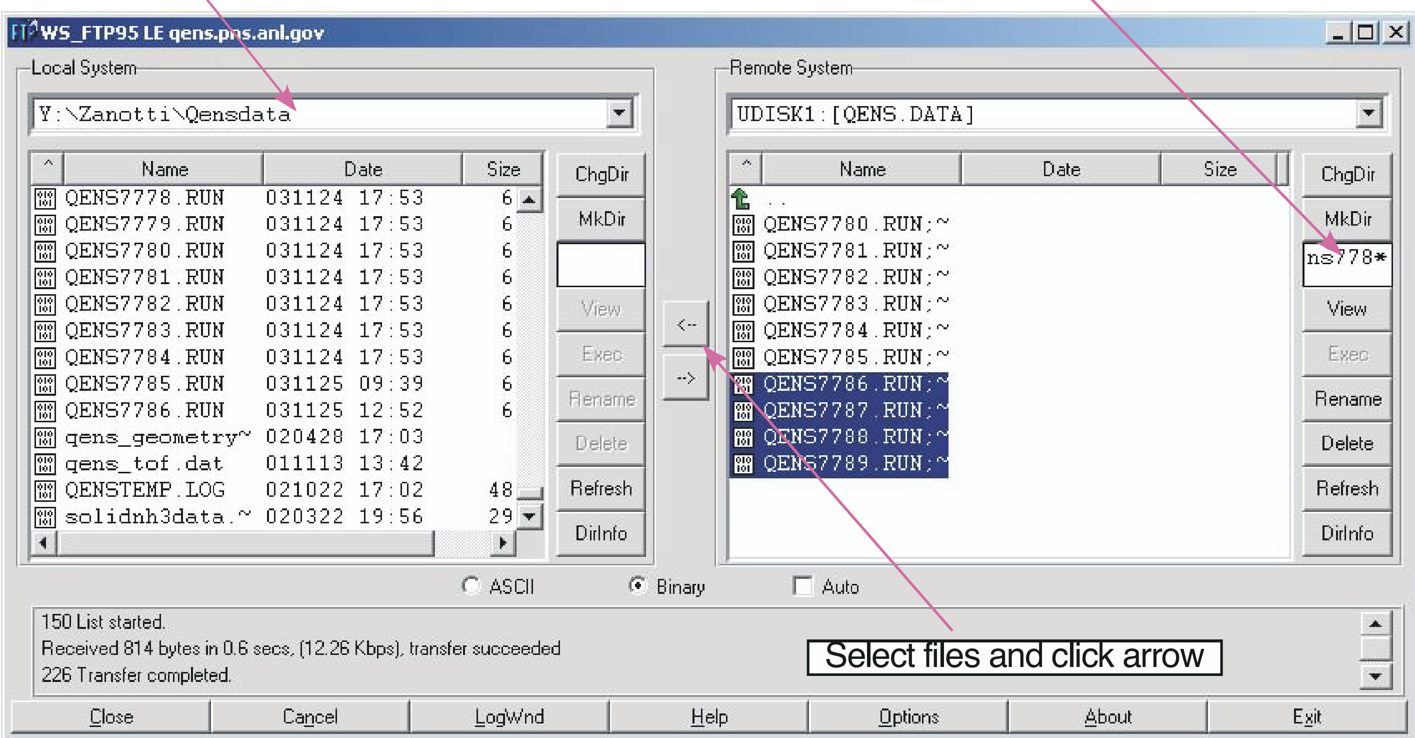
QENS is scheduled for an upgrade to new electronics and DAS in the near future. The new DAS - *Integrated Spectral Analysis Workbench (ISAW)* - is a Java-based, platform-independent, Internet accessible, fully portable and highly interactive software package which has been successfully in operation on some of the IPNS modernized instruments. The new hardware will enhance the performance and capabilities of the detectors, sample environment control, and execution of runs.

The QENS data treatment software is based on IDL which is available via a multi-user license for the local IPNS networked PCs. Look for the QENS User PC in the User Room which should have the necessary data mapping and preferences set up already for analysis of QENS data. *Since the number of concurrent IDL users is limited,* please do not leave IDL idle on the computer. Exit IDL after use.

First, FTP the raw data qensxxxx.run run files from the QENS front-end computer to the PC using WS_FTP95LE (a shortcut on the desktop).

Type a starting string (e.g, qens778* if you want to transfer qens7785.run), then click the Data folder. This will enable a quick look up of the correct runfiles

Data are store in Y:\Zanotti\Qensdata

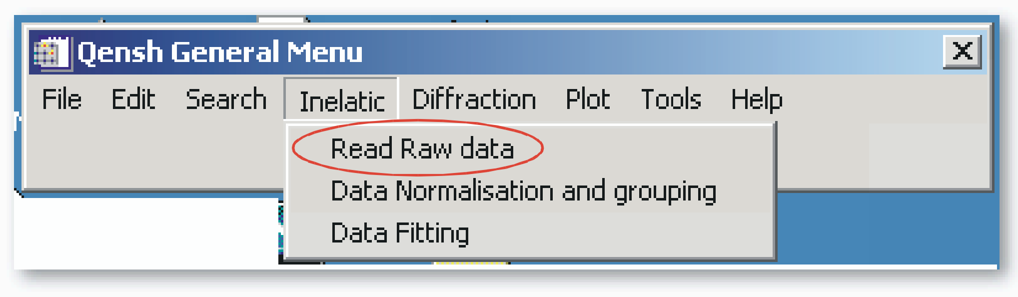


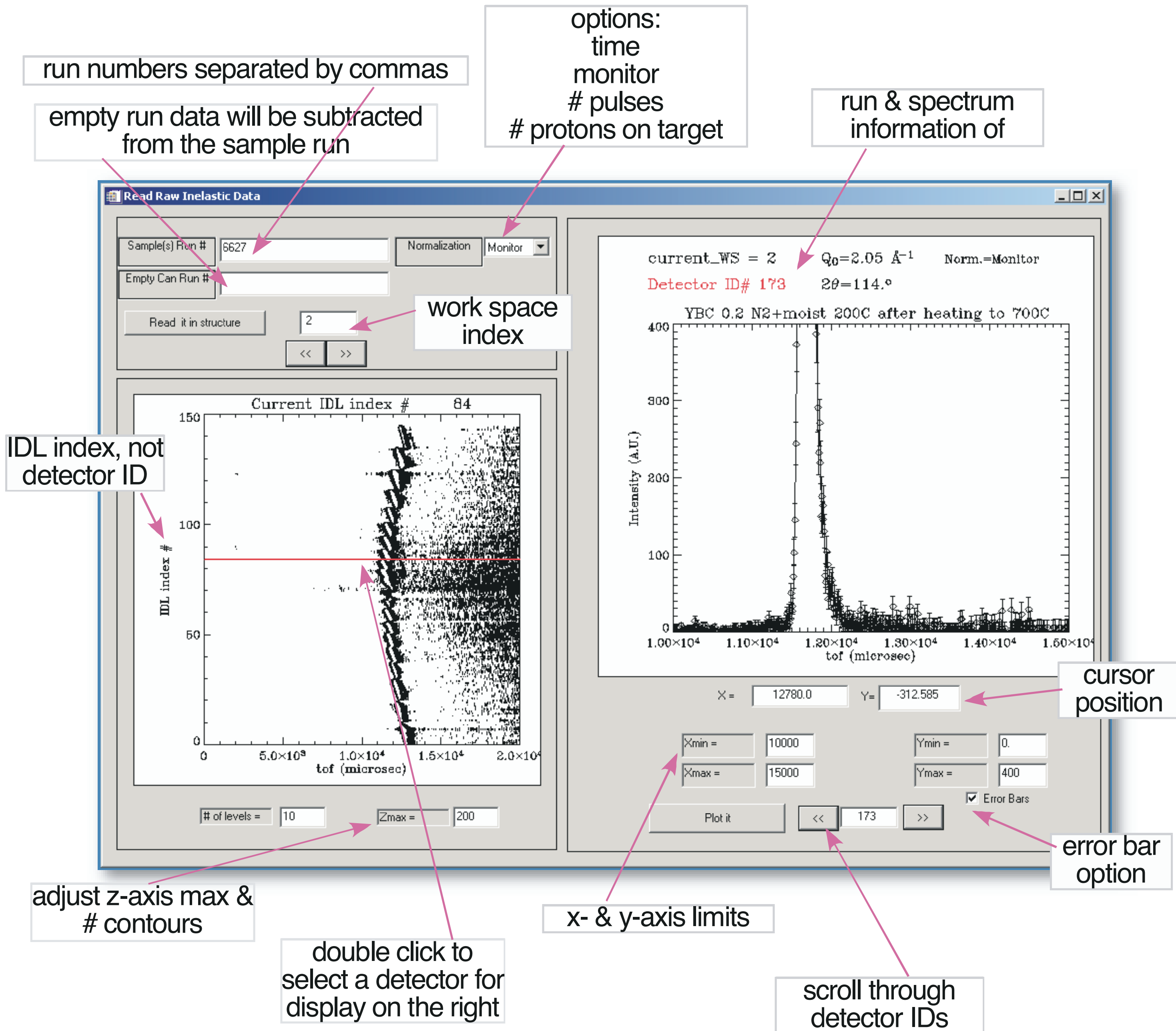
Select files and click arrow

To start IDL, double click the IDL logo, type qensh in the command window.

Check Inelastic Data

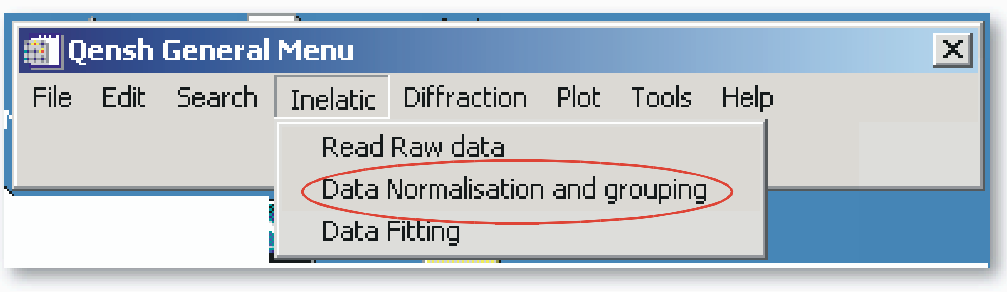
Select `Inelastic>Read Raw data` from the Quesh General Menu. Enter the run number(s) of sample run, select normalization option and an index of the structure (work space) for the data storage in memory.





Calibration & Normalization of Inelastic Data

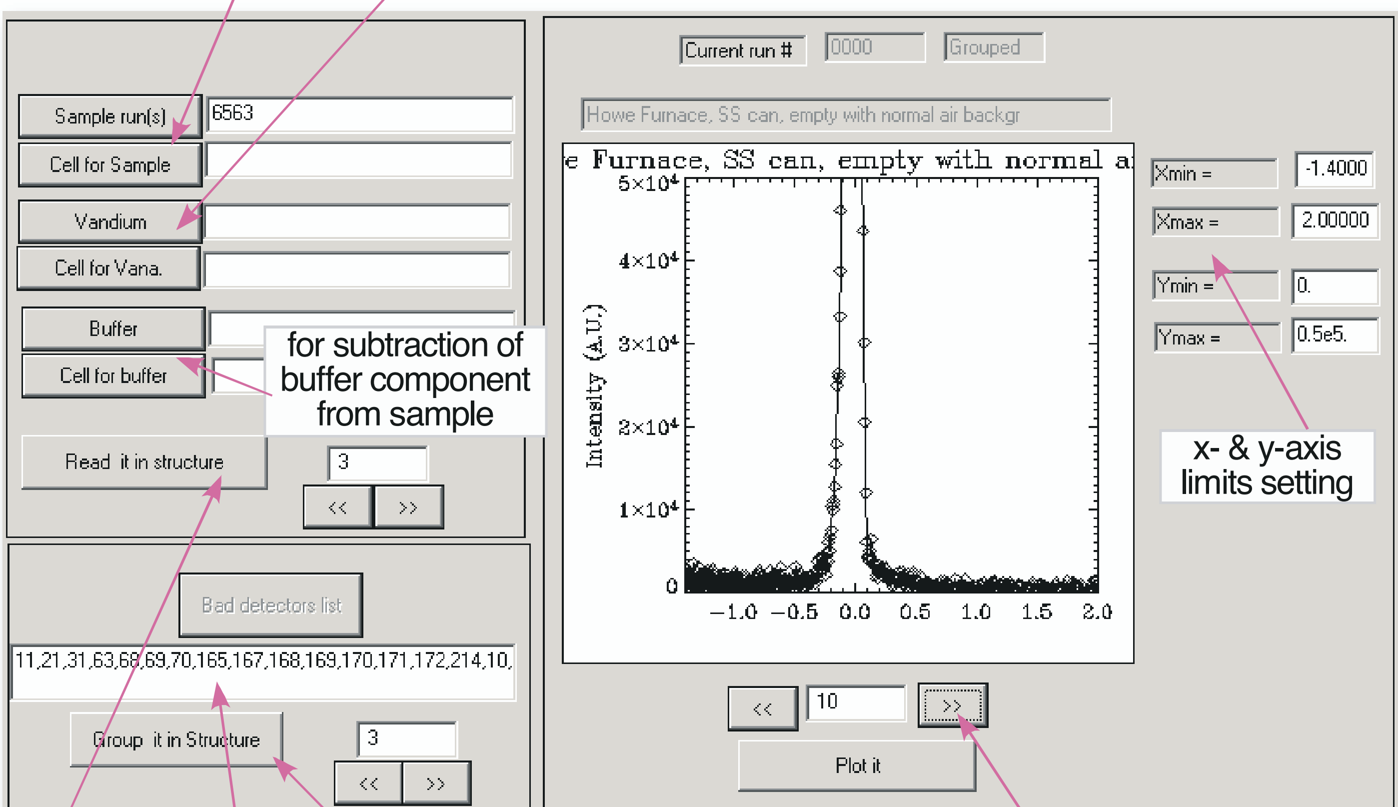
Select `Inelastic>Data Normalization and grouping` from the Quesh General Menu.



You may use this window many times to generate energy-calibrated, detector-efficiency-normalized datasets in different memory workspace for further comparison or treatment later.

run numbers separated by commas; empty run(s), if given, will be subtracted from data

vanadium run(s), if given, will be used to normalize data according to detector efficiencies



for subtraction of buffer component from sample

x- & y-axis limits setting

Generate spectra from individual detectors in memory workspace

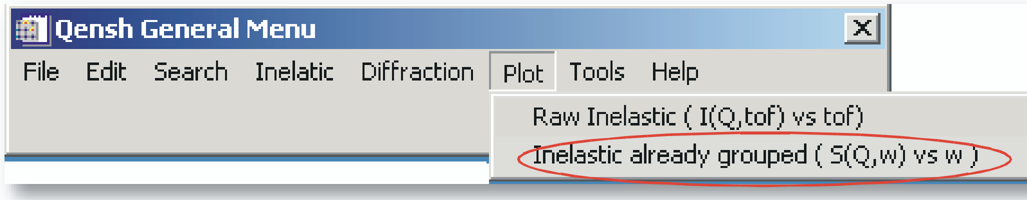
Generate spectra grouped according to detector arms in memory workspace

Scroll spectra through detectors or groups

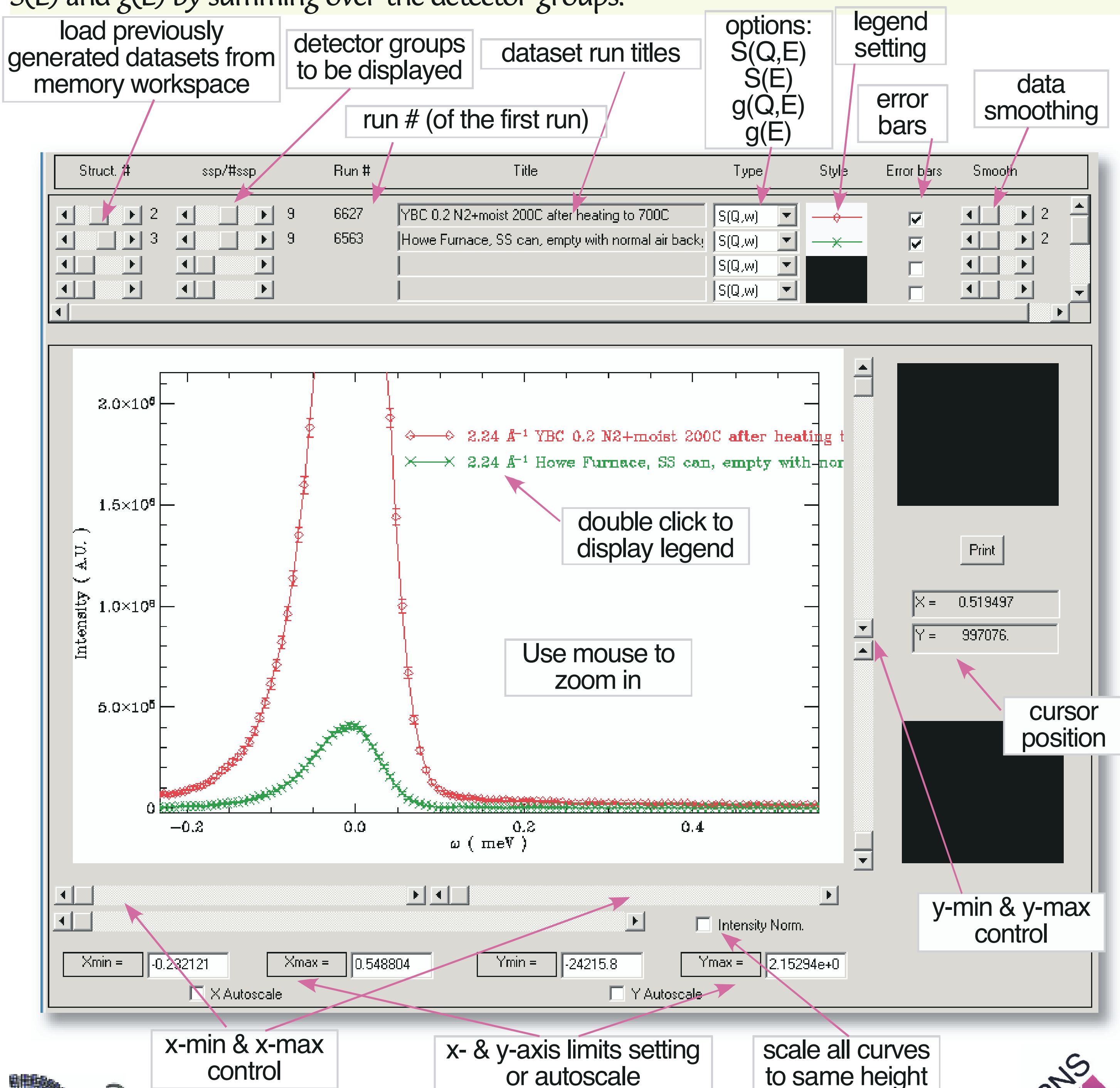
May edit bad-detector list to eliminate them from data

Convert, Integrate, and Overplot Inelastic Datasets

Select `Plot>Inelastic already grouped...` from the Quesh General Menu.

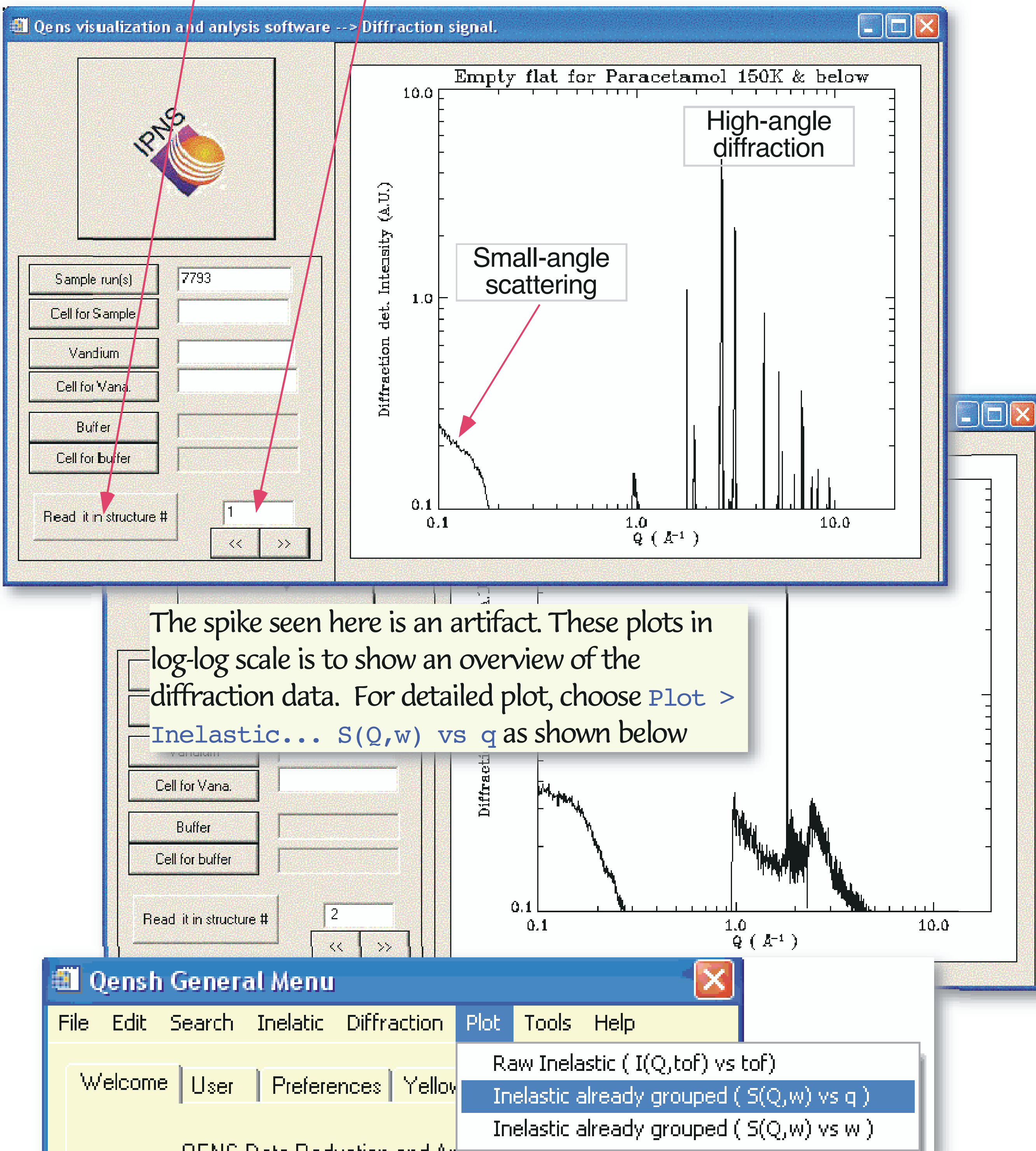


This GUI displays the previously generated datasets from memory workspace as the full structure factor S(ϕ,E) (ϕ is the scattering angle) or the vibrational density of states g(ϕ, E), or S(E) and g(E) by summing over the detector groups.



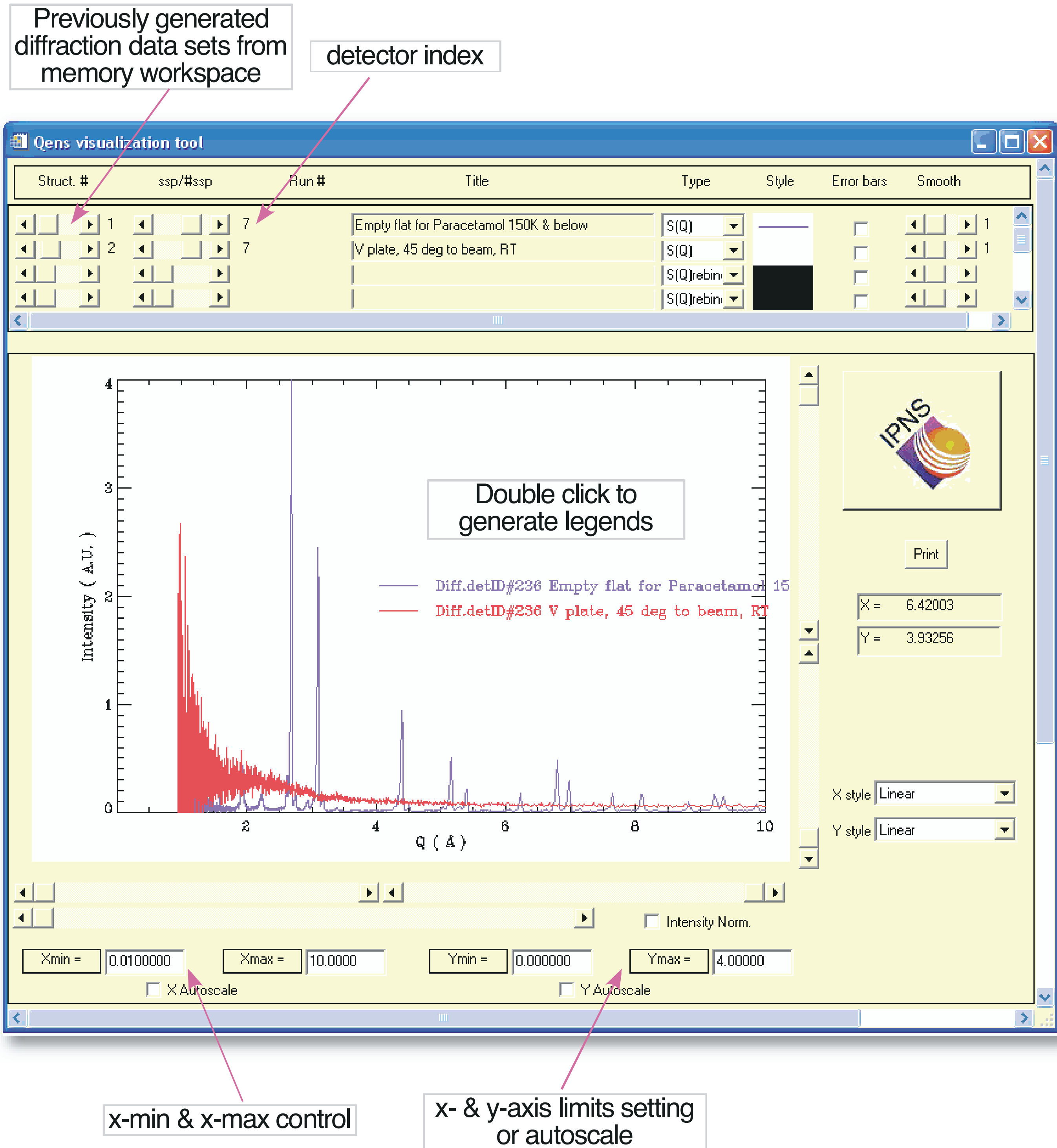
Check Diffraction Data

Select `diffraction > Read Data` from the Quesh General Menu. Enter the run number and an index of the structure (work space) for the diffraction data storage in memory. Click the "Read in Structure #" box.



The spike seen here is an artifact. These plots in log-log scale is to show an overview of the diffraction data. For detailed plot, choose `Plot > Inelastic... S(Q,w) vs q` as shown below

View and Overplot Diffraction Data



ASCII Files of Diffraction & Inelastic Data

ASCII files of $S(Q)$, S(detector arm, E), $S_{sum}(E)$ and $G_{sum}(E)$ are automatically generated whenever `Plot>...` is executed. The files are stored in Y:\Zanotti\QENS\datatreatment\. For example:

Name	Size	Type
Qens_diffraction_7749-n_-.dat	891 KB	DAT F
Qens_diffraction_7793-n_-.dat	890 KB	DAT F
Qens_u2_7743-n-.dat	1 KB	DAT F
Qens_SQW_7743-n-.dat	821 KB	DAT F
Qens_gw_7743-n-.dat	167 KB	DAT F
Qens_elast_int_7743-n-.dat	2 KB	DAT F
Qens_u2_7743-n7743-.dat	1 KB	DAT F
Qens_SQW_7743-n7743-.dat	821 KB	DAT F
Qens_gw_7743-n7743-.dat	167 KB	DAT F
Qens_elast_int_7743-n7743-.dat	2 KB	DAT F
Qens_eff_7743.dat	14 KB	DAT F
Qens_SQW_7793-n-.dat	821 KB	DAT F
Qens_u2_7793-n-.dat	1 KB	DAT F

Data columns: For diffraction:

```
q_4345,dspacing_4345,sq_4345,esq_4345,q_sa_4345,d_sa_4345,sq_sa_4345,sqsa_ns5_4345,
sqsa_ns10_4345,q_ha_4345,d_ha_4345,sq_ha_4345,sqha_ns5_4345,sqha_ns10_4345,qb_4345,
db_4345,sqb_4345
```

correspond to: Q (Å^{-1}), d-spacing (Å), $S(Q)$, $S(Q)$-error, ...
and `sa/ha` designates the sum over the small/high-angle detectors
`nsx,..` are data smooth over x points
`qb,...` are rebinned data of all detectors according to the common Q values.

For inelastic data:

```
w (meV),   d_0_0.36_A-1,   e_0_0.36_A-1,   d_1_0.36_A-1,   e_1_0.36_A-1 ...
```

correspond to E (meV), S(E) for det group 0 with elastic Q of 0.36 Å^{-1}, S(E)-err...., etc.